



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:23 AM UTC

PDB ID : 4TZZ / pdb_00004tzz
Title : Co-crystals of the Ternary Complex Containing a T-box Stem I RNA, its Cognate tRNAGly, and B. subtilis YbxF protein, treated by removing lithium sulfate and increasing PEG3350 concentration from 20% to 45% post crystallization
Authors : Zhang, J.; Ferre-D'Amare, A.R.
Deposited on : 2014-07-11
Resolution : 3.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

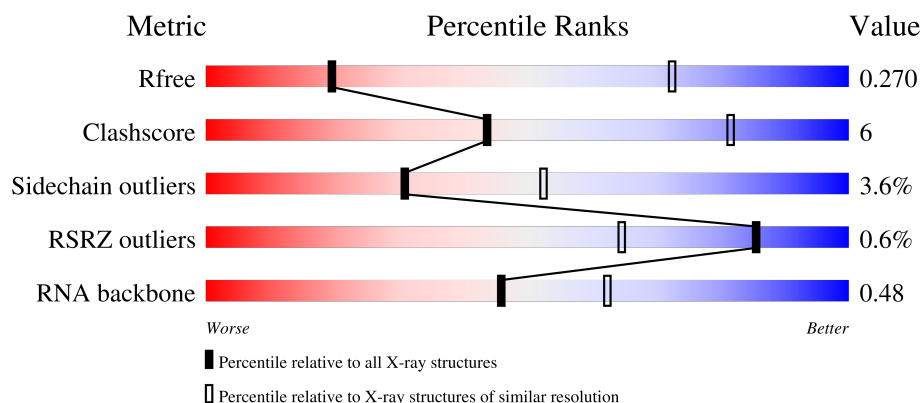
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)
RNA backbone	3983	1026 (4.22-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	82	 2% 76% 21% ..
1	D	82	 4% 70% 27% ..
1	G	82	 % 72% 27% .
1	J	82	 80% 16% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	75	
2	E	75	
2	H	75	
2	K	75	
3	C	102	
3	F	102	
3	I	102	
3	L	102	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17274 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ribosome-associated protein L7Ae-like.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	S	Se	0	0	0
			524	328	88	105	1	2			
1	D	81	Total	C	N	O	S	Se	0	0	0
			524	328	88	105	1	2			
1	G	81	Total	C	N	O	S	Se	0	0	0
			524	328	88	105	1	2			
1	J	81	Total	C	N	O	S	Se	0	0	0
			524	328	88	105	1	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P46350
D	1	GLY	-	expression tag	UNP P46350
G	1	GLY	-	expression tag	UNP P46350
J	1	GLY	-	expression tag	UNP P46350

- Molecule 2 is a RNA chain called engineered tRNAGly.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	75	Total	C	N	O	P	0	0	0
			1592	708	289	520	75			
2	E	75	Total	C	N	O	P	0	0	0
			1592	708	289	520	75			
2	H	75	Total	C	N	O	P	0	0	0
			1592	708	289	520	75			
2	K	75	Total	C	N	O	P	0	0	0
			1591	708	288	520	75			

- Molecule 3 is a RNA chain called T-box Stem I RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	102	Total	C	N	O	P	0	0	0
			2194	982	411	700	101			
3	F	102	Total	C	N	O	P	0	0	0
			2197	982	411	702	102			
3	I	102	Total	C	N	O	P	0	0	0
			2197	982	411	702	102			
3	L	102	Total	C	N	O	P	0	0	0
			2194	982	411	700	101			

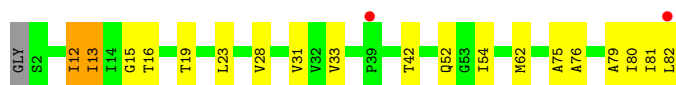
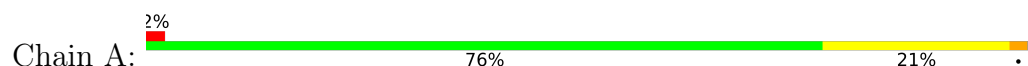
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	C	4	Total	Mg	0	0
			4	4		
4	E	7	Total	Mg	0	0
			7	7		
4	F	4	Total	Mg	0	0
			4	4		
4	H	5	Total	Mg	0	0
			5	5		
4	I	5	Total	Mg	0	0
			5	5		
4	L	2	Total	Mg	0	0
			2	2		

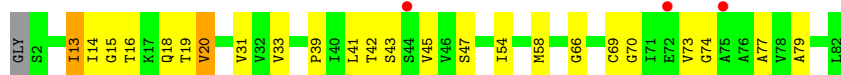
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ribosome-associated protein L7Ae-like



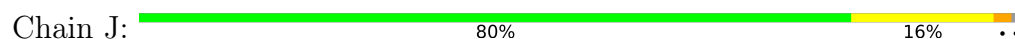
- Molecule 1: Ribosome-associated protein L7Ae-like



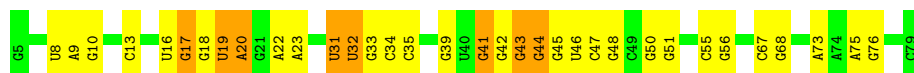
- Molecule 1: Ribosome-associated protein L7Ae-like



- Molecule 1: Ribosome-associated protein L7Ae-like

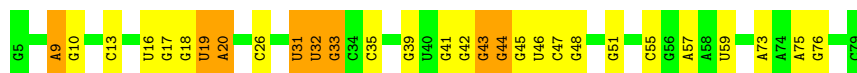


- Molecule 2: engineered tRNA^{Gly}



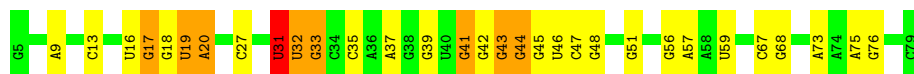
- Molecule 2: engineered tRNA^{Gly}

Chain E:  61% 28% 11%



- Molecule 2: engineered tRNA^{Gly}

Chain H:  59% 29% 11%



- Molecule 2: engineered tRNA^{Gly}

Chain K:  60% 29% 11%



- Molecule 3: T-box Stem I RNA

Chain C:  65% 29% 6%



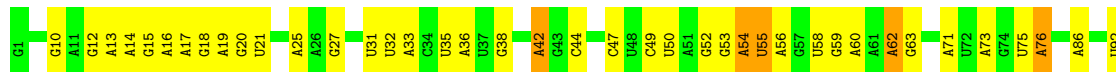
- Molecule 3: T-box Stem I RNA

Chain F:  64% 31% 5%



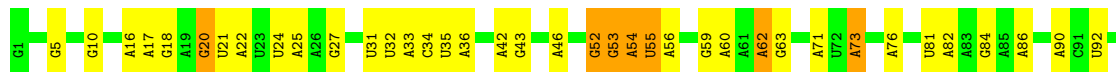
- Molecule 3: T-box Stem I RNA

Chain I:  58% 37% 5%



- Molecule 3: T-box Stem I RNA

Chain L:  62% 31% 7%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.64Å 260.73Å 70.70Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	70.61 – 3.64 70.61 – 3.64	Depositor EDS
% Data completeness (in resolution range)	84.1 (70.61-3.64) 84.0 (70.61-3.64)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.217 , 0.269 0.220 , 0.270	Depositor DCC
R_{free} test set	1230 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	147.8	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 251.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.076 for l,k,-h 0.096 for h,-k,-l 0.137 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17274	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/523	0.87	0/709
1	D	0.36	0/523	0.92	1/709 (0.1%)
1	G	0.33	0/523	0.89	2/709 (0.3%)
1	J	0.30	0/523	0.81	0/709
2	B	0.10	0/1780	0.27	0/2775
2	E	0.10	0/1780	0.28	0/2775
2	H	0.10	0/1780	0.28	1/2775 (0.0%)
2	K	0.10	0/1779	0.27	0/2773
3	C	0.09	0/2461	0.21	0/3838
3	F	0.09	0/2464	0.22	0/3842
3	I	0.09	0/2464	0.22	0/3842
3	L	0.09	0/2461	0.21	0/3838
All	All	0.14	0/19061	0.36	4/29294 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	38	ASP	CA-C-N	5.22	125.30	119.87
1	G	38	ASP	C-N-CA	5.22	125.30	119.87
1	D	70	GLY	N-CA-C	-5.22	108.43	115.21
2	H	31	U	P-O3'-C3'	5.17	127.96	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	524	0	505	10	0
1	D	524	0	505	14	0
1	G	524	0	505	13	0
1	J	524	0	505	8	0
2	B	1592	0	804	14	0
2	E	1592	0	804	13	0
2	H	1592	0	804	12	0
2	K	1591	0	802	12	0
3	C	2194	0	1100	14	0
3	F	2197	0	1100	17	0
3	I	2197	0	1098	16	0
3	L	2194	0	1101	20	0
4	B	2	0	0	0	0
4	C	4	0	0	0	0
4	E	7	0	0	0	0
4	F	4	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	L	2	0	0	0	0
All	All	17274	0	9633	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:10:G:N7	2:K:44:G:N2	2.23	0.87
2:K:32:U:O2'	2:K:34:C:OP2	1.95	0.83
3:L:35:U:H3	3:L:73:A:H61	1.33	0.76
2:H:31:U:H4'	2:H:32:U:O5'	1.84	0.76
2:E:32:U:H4'	2:E:33:G:OP1	1.84	0.76
3:I:59:G:N1	3:I:62:A:OP2	2.21	0.73
2:B:10:G:N7	2:B:44:G:N2	2.37	0.71
1:D:18:GLN:NE2	3:F:95:G:OP2	2.22	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:13:ILE:HG22	1:J:79:ALA:HB3	1.73	0.70
2:K:32:U:O2'	2:K:33:G:OP1	2.11	0.69
2:B:17:G:O2'	2:B:56:G:N2	2.23	0.69
1:D:66:GLY:HA3	1:D:74:GLY:HA2	1.75	0.67
1:D:39:PRO:HA	1:D:42:THR:HB	1.75	0.67
1:G:19:THR:HG23	1:G:79:ALA:HB2	1.76	0.67
3:L:5:G:H1	3:L:98:C:H42	1.41	0.67
2:B:31:U:H4'	2:B:32:U:O5'	1.94	0.67
2:K:17:G:O2'	2:K:56:G:N2	2.28	0.66
1:J:66:GLY:HA3	1:J:74:GLY:HA2	1.78	0.66
1:G:66:GLY:HA3	1:G:74:GLY:HA2	1.81	0.63
1:D:13:ILE:HG22	1:D:79:ALA:HB3	1.79	0.63
1:A:28:VAL:HA	1:A:81:ILE:HA	1.81	0.61
1:A:13:ILE:HG22	1:A:79:ALA:HB3	1.83	0.61
2:E:31:U:H4'	2:E:32:U:OP1	2.01	0.60
1:A:31:VAL:HG23	1:A:54:ILE:HD13	1.82	0.60
2:E:10:G:N7	2:E:44:G:N2	2.48	0.60
3:F:59:G:N1	3:F:62:A:OP2	2.36	0.58
3:I:19:A:OP1	3:I:21:U:H1'	2.03	0.58
3:I:54:A:H1'	3:I:55:U:H5'	1.85	0.57
3:C:28:G:H1	3:C:78:C:H42	1.52	0.57
3:F:42:A:H62	3:F:46:A:H62	1.51	0.57
1:D:16:THR:HA	1:D:77:ALA:HB3	1.87	0.56
2:H:17:G:O2'	2:H:56:G:N2	2.30	0.56
3:L:16:A:H61	3:L:90:A:H61	1.52	0.56
1:G:39:PRO:HA	1:G:42:THR:HB	1.87	0.55
1:D:15:GLY:O	1:D:19:THR:HG23	2.07	0.55
2:B:32:U:O2'	2:B:34:C:OP2	2.13	0.55
3:F:54:A:H1'	3:F:55:U:H5'	1.89	0.55
3:C:25:A:H61	3:C:81:U:H3	1.53	0.55
3:L:18:G:H2'	3:L:86:A:H61	1.72	0.55
3:I:35:U:H2'	3:I:36:A:C8	2.43	0.54
3:L:54:A:H2'	3:L:54:A:OP2	2.07	0.54
1:D:41:LEU:HD21	3:F:10:G:N7	2.23	0.53
1:J:30:GLU:HG2	1:J:80:ILE:HD12	1.91	0.53
3:F:45:G:N2	3:F:62:A:O2'	2.42	0.53
1:G:10:LYS:H	1:G:82:LEU:HD21	1.75	0.52
3:F:21:U:H2'	3:F:22:A:H8	1.74	0.52
2:E:42:G:HO2'	2:E:43:G:H8	1.54	0.51
2:K:42:G:HO2'	2:K:43:G:H8	1.57	0.51
2:E:19:U:H1'	2:E:20:A:OP2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:42:G:O2'	2:E:43:G:H8	1.93	0.51
2:H:32:U:H4'	2:H:33:G:OP2	2.11	0.51
1:G:30:GLU:HG2	1:G:80:ILE:HD12	1.93	0.50
3:I:38:G:N3	3:I:47:C:H5'	2.26	0.50
2:B:75:A:C5	2:B:76:G:H1'	2.47	0.50
1:D:20:VAL:HG23	1:D:45:VAL:HG23	1.94	0.50
2:H:31:U:H3	2:H:37:A:H61	1.59	0.50
3:I:42:A:H2'	3:I:58:U:O2'	2.11	0.50
2:H:43:G:H1'	2:H:44:G:H5'	1.94	0.50
3:C:54:A:H1'	3:C:55:U:H5'	1.93	0.49
2:E:9:A:O2'	2:E:10:G:N7	2.45	0.49
2:K:42:G:O2'	2:K:43:G:H8	1.95	0.49
3:C:54:A:H2'	3:C:54:A:OP2	2.11	0.49
1:J:80:ILE:HG22	1:J:82:LEU:HG	1.93	0.49
2:E:75:A:C5	2:E:76:G:H1'	2.48	0.49
2:K:9:A:O2'	2:K:10:G:N7	2.46	0.49
2:B:42:G:O2'	2:B:43:G:H8	1.96	0.49
3:I:18:G:H2'	3:I:86:A:H61	1.77	0.48
1:A:15:GLY:O	1:A:19:THR:HG23	2.14	0.48
1:D:43:SER:O	1:D:47:SER:HB3	2.14	0.48
3:I:15:G:H2'	3:I:16:A:H8	1.78	0.48
3:F:42:A:H2'	3:F:58:U:O2'	2.14	0.48
2:K:31:U:H3	2:K:37:A:H61	1.62	0.47
3:L:18:G:H2'	3:L:86:A:N6	2.28	0.47
3:C:42:A:H2'	3:C:58:U:O2'	2.14	0.47
3:I:54:A:OP2	3:I:54:A:H2'	2.14	0.47
3:I:15:G:H2'	3:I:16:A:C8	2.50	0.47
1:J:16:THR:HG21	1:J:41:LEU:HG	1.97	0.47
2:K:75:A:C5	2:K:76:G:H1'	2.50	0.46
2:E:20:A:H2'	2:E:20:A:OP1	2.15	0.46
2:K:8:U:O2'	2:K:20:A:N1	2.39	0.46
2:B:50:G:H5''	2:E:26:C:H5''	1.97	0.46
3:L:24:U:H3	3:L:82:A:H61	1.62	0.46
3:I:49:C:H2'	3:I:50:U:C6	2.50	0.46
2:B:8:U:O2'	2:B:20:A:N1	2.47	0.46
3:C:38:G:N3	3:C:47:C:H5'	2.30	0.46
1:D:73:VAL:HG21	3:F:7:G:N1	2.30	0.46
3:L:53:G:H3'	3:L:54:A:H8	1.81	0.46
1:A:23:LEU:O	1:A:52:GLN:NE2	2.49	0.46
2:H:57:A:O2'	2:H:59:U:OP2	2.31	0.46
1:A:62:MSE:HB2	1:A:75:ALA:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:A:O2'	2:E:59:U:OP2	2.33	0.45
2:B:19:U:H1'	2:B:20:A:OP2	2.16	0.45
3:F:22:A:H2'	3:F:23:U:O4'	2.17	0.45
2:K:7:G:O2'	2:K:48:G:O5'	2.34	0.45
1:A:33:VAL:HG11	1:A:42:THR:HG23	1.99	0.45
1:D:31:VAL:HG23	1:D:54:ILE:HD13	1.99	0.45
1:A:80:ILE:HG22	1:A:82:LEU:HG	1.99	0.45
1:D:13:ILE:CG2	1:D:79:ALA:HB3	2.47	0.45
2:B:32:U:H2'	2:B:32:U:OP2	2.17	0.44
3:C:15:G:H2'	3:C:16:A:C8	2.52	0.44
2:H:42:G:O2'	2:H:43:G:H8	2.00	0.44
2:H:75:A:C5	2:H:76:G:H1'	2.53	0.44
3:L:52:G:C2	3:L:53:G:H1'	2.51	0.44
3:L:59:G:N1	3:L:62:A:OP2	2.51	0.44
2:B:55:C:O2'	3:C:55:U:H5''	2.18	0.44
2:H:19:U:H1'	2:H:20:A:OP2	2.17	0.44
2:B:22:A:H2'	2:B:23:A:C8	2.53	0.44
1:D:14:ILE:HG12	1:D:69:CYS:HB3	2.00	0.44
1:G:3:TYR:OH	1:G:61:SER:N	2.35	0.44
1:G:28:VAL:HA	1:G:81:ILE:HA	2.00	0.43
1:G:33:VAL:HG11	1:G:42:THR:HG23	2.00	0.43
3:I:13:A:H2'	3:I:14:A:C8	2.53	0.43
3:L:54:A:H1'	3:L:55:U:H5'	1.99	0.43
3:I:98:C:H2'	3:I:99:A:C8	2.54	0.43
3:L:5:G:H1	3:L:98:C:N4	2.14	0.43
3:C:35:U:H2'	3:C:36:A:C8	2.53	0.43
3:I:44:C:H42	3:I:63:G:H1	1.65	0.43
3:F:81:U:H2'	3:F:82:A:C8	2.53	0.43
2:H:27:C:H42	2:H:41:G:H1	1.67	0.43
3:I:75:U:O4	3:I:76:A:N6	2.53	0.42
1:J:15:GLY:O	1:J:19:THR:HG23	2.18	0.42
3:C:59:G:N1	3:C:62:A:OP2	2.52	0.42
1:G:59:VAL:HG21	1:G:65:LEU:HD22	2.01	0.42
3:L:20:G:O2'	3:L:84:G:O6	2.28	0.42
1:D:33:VAL:O	1:D:58:MSE:HA	2.19	0.42
2:H:67:C:H2'	2:H:68:G:C8	2.54	0.42
3:L:16:A:H61	3:L:90:A:N6	2.17	0.42
1:G:49:ALA:O	1:G:54:ILE:HG22	2.19	0.42
1:J:21:LYS:O	1:J:25:ARG:HG2	2.20	0.42
1:A:12:ILE:HG22	1:A:80:ILE:HG12	2.02	0.42
3:F:21:U:H2'	3:F:22:A:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:35:U:H2'	3:L:36:A:C8	2.55	0.42
3:L:81:U:H2'	3:L:82:A:C8	2.55	0.42
1:G:6:VAL:HG21	1:G:65:LEU:HD11	2.02	0.42
3:I:12:G:N2	3:I:94:C:O2	2.40	0.42
3:L:81:U:H2'	3:L:82:A:H8	1.85	0.42
2:B:67:C:H2'	2:B:68:G:C8	2.55	0.41
3:C:43:G:O2'	3:C:57:G:N2	2.52	0.41
2:E:55:C:O2'	3:F:55:U:H5''	2.19	0.41
1:J:33:VAL:HG11	1:J:42:THR:HG23	2.01	0.41
2:E:42:G:O2'	2:E:43:G:H5'	2.20	0.41
3:F:35:U:H2'	3:F:36:A:C8	2.55	0.41
2:K:42:G:OP1	3:L:34:C:H5''	2.21	0.41
3:F:49:C:H2'	3:F:50:U:C6	2.56	0.41
3:C:20:G:O2'	3:C:84:G:O6	2.35	0.41
1:A:16:THR:HG23	1:A:76:ALA:HB3	2.03	0.40
3:F:47:C:H1'	3:F:70:G:N2	2.37	0.40
3:F:81:U:H2'	3:F:82:A:H8	1.86	0.40
1:G:28:VAL:HG22	1:G:54:ILE:HD11	2.01	0.40
2:H:31:U:H3	2:H:37:A:N6	2.19	0.40
3:L:21:U:H2'	3:L:22:A:H8	1.86	0.40
3:C:25:A:N6	3:C:81:U:H3	2.19	0.40
1:G:65:LEU:HD12	1:G:65:LEU:HA	1.88	0.40
3:L:43:G:N2	3:L:46:A:OP2	2.52	0.40
2:B:41:G:H5'	3:C:34:C:H4'	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	48/63 (76%)	46 (96%)	2 (4%)	26	49
1	D	48/63 (76%)	46 (96%)	2 (4%)	26	49
1	G	48/63 (76%)	47 (98%)	1 (2%)	47	62
1	J	48/63 (76%)	46 (96%)	2 (4%)	26	49
All	All	192/252 (76%)	185 (96%)	7 (4%)	31	52

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	13	ILE
1	D	13	ILE
1	D	20	VAL
1	G	40	ILE
1	J	13	ILE
1	J	16	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	8	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	74/75 (98%)	20 (27%)	2 (2%)
2	E	74/75 (98%)	20 (27%)	3 (4%)
2	H	74/75 (98%)	20 (27%)	3 (4%)
2	K	74/75 (98%)	20 (27%)	2 (2%)
3	C	101/102 (99%)	21 (20%)	0
3	F	101/102 (99%)	20 (19%)	0
3	I	101/102 (99%)	20 (19%)	0
3	L	101/102 (99%)	21 (20%)	0
All	All	700/708 (98%)	162 (23%)	10 (1%)

All (162) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	13	C
2	B	16	U
2	B	17	G
2	B	18	G
2	B	19	U
2	B	20	A
2	B	32	U
2	B	33	G
2	B	35	C
2	B	39	G
2	B	41	G
2	B	43	G
2	B	44	G
2	B	45	G
2	B	46	U
2	B	47	C
2	B	48	G
2	B	51	G
2	B	73	A
3	C	10	G
3	C	17	A
3	C	20	G
3	C	25	A
3	C	27	G
3	C	31	U
3	C	32	U
3	C	33	A
3	C	42	A
3	C	52	G
3	C	53	G
3	C	54	A
3	C	55	U
3	C	56	A
3	C	60	A
3	C	62	A
3	C	63	G
3	C	71	A
3	C	73	A
3	C	76	A
3	C	92	U
2	E	9	A
2	E	13	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	16	U
2	E	17	G
2	E	18	G
2	E	19	U
2	E	20	A
2	E	32	U
2	E	33	G
2	E	35	C
2	E	39	G
2	E	41	G
2	E	43	G
2	E	44	G
2	E	45	G
2	E	46	U
2	E	47	C
2	E	48	G
2	E	51	G
2	E	73	A
3	F	10	G
3	F	17	A
3	F	20	G
3	F	25	A
3	F	27	G
3	F	31	U
3	F	32	U
3	F	33	A
3	F	42	A
3	F	52	G
3	F	53	G
3	F	54	A
3	F	55	U
3	F	56	A
3	F	60	A
3	F	62	A
3	F	71	A
3	F	73	A
3	F	76	A
3	F	92	U
2	H	9	A
2	H	13	C
2	H	16	U
2	H	17	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	18	G
2	H	19	U
2	H	20	A
2	H	32	U
2	H	33	G
2	H	35	C
2	H	39	G
2	H	41	G
2	H	43	G
2	H	44	G
2	H	45	G
2	H	46	U
2	H	47	C
2	H	48	G
2	H	51	G
2	H	73	A
3	I	10	G
3	I	17	A
3	I	20	G
3	I	25	A
3	I	27	G
3	I	31	U
3	I	32	U
3	I	33	A
3	I	42	A
3	I	52	G
3	I	53	G
3	I	54	A
3	I	55	U
3	I	56	A
3	I	60	A
3	I	62	A
3	I	71	A
3	I	73	A
3	I	76	A
3	I	92	U
2	K	9	A
2	K	13	C
2	K	16	U
2	K	17	G
2	K	18	G
2	K	19	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	20	A
2	K	32	U
2	K	33	G
2	K	35	C
2	K	39	G
2	K	41	G
2	K	43	G
2	K	44	G
2	K	45	G
2	K	46	U
2	K	47	C
2	K	48	G
2	K	51	G
2	K	73	A
3	L	10	G
3	L	17	A
3	L	20	G
3	L	25	A
3	L	27	G
3	L	31	U
3	L	32	U
3	L	33	A
3	L	42	A
3	L	52	G
3	L	53	G
3	L	54	A
3	L	55	U
3	L	56	A
3	L	60	A
3	L	62	A
3	L	63	G
3	L	71	A
3	L	73	A
3	L	76	A
3	L	92	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	19	U
2	B	31	U
2	E	19	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	31	U
2	E	32	U
2	H	19	U
2	H	31	U
2	H	32	U
2	K	19	U
2	K	32	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 29 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	79/82 (96%)	-0.26	2 (2%) 58 35	102, 170, 227, 242	0
1	D	79/82 (96%)	0.50	3 (3%) 44 26	146, 273, 306, 334	0
1	G	79/82 (96%)	-0.32	1 (1%) 75 49	62, 105, 160, 170	0
1	J	79/82 (96%)	-0.18	0 100 100	93, 143, 193, 211	0
2	B	75/75 (100%)	-0.76	0 100 100	73, 101, 125, 139	0
2	E	75/75 (100%)	-0.72	0 100 100	61, 81, 146, 192	0
2	H	75/75 (100%)	-0.82	0 100 100	57, 100, 139, 152	0
2	K	75/75 (100%)	-0.82	0 100 100	60, 87, 129, 165	0
3	C	102/102 (100%)	-0.92	0 100 100	69, 99, 123, 144	0
3	F	102/102 (100%)	-0.76	0 100 100	63, 116, 170, 197	0
3	I	102/102 (100%)	-0.74	0 100 100	63, 116, 163, 220	0
3	L	102/102 (100%)	-0.60	0 100 100	82, 144, 196, 217	0
All	All	1024/1036 (98%)	-0.55	6 (0%) 85 65	57, 114, 242, 334	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	70	GLY	3.6
1	D	72	GLU	3.3
1	D	75	ALA	3.3
1	D	44	SER	3.3
1	A	39	PRO	2.5
1	A	82	LEU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	H	102	1/1	0.73	0.14	96,96,96,96	0
4	MG	E	102	1/1	0.90	0.15	93,93,93,93	0
4	MG	B	101	1/1	0.92	0.20	77,77,77,77	0
4	MG	E	103	1/1	0.92	0.18	86,86,86,86	0
4	MG	C	201	1/1	0.92	0.11	49,49,49,49	0
4	MG	E	107	1/1	0.94	0.12	68,68,68,68	0
4	MG	H	104	1/1	0.94	0.17	60,60,60,60	0
4	MG	F	204	1/1	0.95	0.19	86,86,86,86	0
4	MG	F	202	1/1	0.95	0.10	61,61,61,61	0
4	MG	F	203	1/1	0.95	0.08	102,102,102,102	0
4	MG	H	105	1/1	0.95	0.15	91,91,91,91	0
4	MG	I	202	1/1	0.95	0.06	48,48,48,48	0
4	MG	I	204	1/1	0.95	0.09	48,48,48,48	0
4	MG	E	106	1/1	0.96	0.16	92,92,92,92	0
4	MG	E	104	1/1	0.96	0.06	48,48,48,48	0
4	MG	F	201	1/1	0.97	0.09	69,69,69,69	0
4	MG	I	201	1/1	0.97	0.09	66,66,66,66	0
4	MG	H	103	1/1	0.97	0.19	69,69,69,69	0
4	MG	H	101	1/1	0.97	0.14	47,47,47,47	0
4	MG	L	202	1/1	0.97	0.14	68,68,68,68	0
4	MG	E	105	1/1	0.98	0.09	59,59,59,59	0
4	MG	B	102	1/1	0.98	0.13	60,60,60,60	0
4	MG	I	203	1/1	0.98	0.08	72,72,72,72	0
4	MG	C	202	1/1	0.98	0.11	50,50,50,50	0
4	MG	I	205	1/1	0.98	0.06	56,56,56,56	0
4	MG	C	204	1/1	0.98	0.10	58,58,58,58	0
4	MG	E	101	1/1	0.99	0.08	33,33,33,33	0
4	MG	L	201	1/1	0.99	0.06	63,63,63,63	0
4	MG	C	203	1/1	0.99	0.09	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.